

1,4,5,8-Dimethanoanthracene-9,10-diol-1,4,5,8-tetraol

Inchi:	InChI=1S/C16H14O2/c17-15-11-7-1-2-8(5-7)12(11)16(18)14-10-4-3-9(6-10)13(14)15/h1-16
InchiKey:	RBOSFZNDAGQKRM-UHFFFAOYSA-N
Formula:	C16H14O2
SMILES:	Oc1c2c(c(O)c3c1C1C=CC3C1)C1C=CC2C1
Mol. weight [g/mol]:	238.28
CAS:	17694-16-5

Physical Properties

Property code	Value	Unit	Source
gf	185.24	kJ/mol	Joback Method
hf	-106.99	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	81.39	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.379		Crippen Method
mcvol	172.240	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	785.08	K	Joback Method
tc	1038.81	K	Joback Method
tf	637.82	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.75	J/molxK	785.08	Joback Method
cpg	555.29	J/molxK	827.37	Joback Method
cpg	568.83	J/molxK	869.66	Joback Method
cpg	582.77	J/molxK	911.95	Joback Method
cpg	597.50	J/molxK	954.23	Joback Method
cpg	613.40	J/molxK	996.52	Joback Method
cpg	630.87	J/molxK	1038.81	Joback Method
dvisc	0.0003528	Paxs	637.82	Joback Method
dvisc	0.0002790	Paxs	662.36	Joback Method

dvisc	0.0002244	Paxs	686.91	Joback Method
dvisc	0.0001832	Paxs	711.45	Joback Method
dvisc	0.0001516	Paxs	735.99	Joback Method
dvisc	0.0001269	Paxs	760.54	Joback Method
dvisc	0.0001075	Paxs	785.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17694165&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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